4-Hexylresorcinol 136-77-6 | DTXSID1020699

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Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 57.1

Global applicability domain: Inside

Local applicability domain index: 5.02e-01

Confidence level: 6.93e-01

Nearest Neighbors from the Training Set

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1-Ethenoxy-2-ethylhexane

Measured: 603 Predicted: 284 Image not found

Carbaryl

Measured: 8.91 **Predicted:** 5.04

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Tributylamine
Measured: 25.1
Predicted: 23.2

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Isoamyl ether Measured: 170 Predicted: 137 Image not found

Fenobucarb Measured: 25.7 Predicted: 15.9